The Harary index of trees [*]

Aleksandar Ilić [‡]

Faculty of Sciences and Mathematics, University of Niš

Višegradska 33, 18000 Niš, Serbia

e-mail: `aleksandari@gmail.com`

Guihai Yu

Department of Mathematics, Shandong Institute of Business and Technology

191 Binhaizhong Road, Yantai, Shandong, P.R. China, 264005.

e-mail: `yuguihai@126.com`

Lihua Feng

Department of Mathematics, Central South University

Railway Campus, Changsha, Hunan, P. R. China, 410075.

e-mail: `fenglh@163.com`

January 19, 2013

Abstract

The Harary index of a graph G is recently introduced topological index, defined on the reverse distance matrix as $H(G) = \sum_{u,v \in V(G)} \frac{1}{d(u,v)}$, where $d(u,v)$ is the length of the shortest path between two distinct vertices u and v. We present the partial ordering of starlike trees based on the Harary index and we describe the trees with the second maximal and the second minimal Harary index. In this paper, we investigate the Harary index of trees with k pendent vertices and determine the extremal trees with maximal Harary index. We also characterize the extremal trees with maximal Harary index with respect to the number of vertices of degree two, matching number, independence number, radius and diameter. In addition, we characterize the extremal trees with minimal Harary index and given maximum degree. We concluded that in all presented classes, the trees with maximal Harary index are exactly those trees with the minimal Wiener index, and vice versa.

AMS Classifications: 92E10, 05C12.

1   Introduction

In theoretical chemistry molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [23, 24]. There exist several types of such indices, especially those based on graph-theoretical distances.

In 1993 Plavšić et al. in [22] and Ivanciuc et al. in [15] independently introduced a new topological index, which was named Harary index in honor of Frank Harary on the occasion of his 70th birthday. This topological index is derived from the reciprocal distance matrix and has a number of interesting chemical-physics properties [16]. The Harary index and its related molecular descriptors have shown some success in structure-property correlations [2, 3, 4, 10, 17, 20, 28]. Its modification has also been proposed [21] and their use in combination with other molecular descriptors improves the correlations [23, 25]. It is of interest to study spectra and polynomials of these matrices [9, 27].

In this paper, let G be a simple connected (molecular) graph with vertex set $V(G)$. The Harary index is defined as the half-sum of the elements in the reciprocal distance matrix (also called the Harary matrix [18]),

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d(u,v)},$$

where $d(u,v)$ is the distance between u and v in G and the sum goes over all the pairs of vertices. The Wiener index, defined as

$$W(G) = \sum_{u,v \in V(G)} d(u,v),$$

is considered as one of the most used topological indices with high correlation with many physical and chemical properties of molecular compounds. The majority of chemical applications of the Wiener index deal with acyclic organic molecules. For recent results and applications of Wiener index see [5].

Up to now, many results were obtained concerning the Harary index of a graph. Gutman [10] supported the use of Harary index as a measure of branching in alkanes, by showing

Theorem 1.1 *Let T be a tree on n vertices. Then*

$$1 + n \sum_{k=2}^{n-1} \frac{1}{k} \leq H(T) \leq \frac{(n+2)(n-1)}{4}.$$

The right equality holds if and only if $T \cong S_n$, while the left equality holds if and only if $T \cong P_n$.

2

In this paper, we further refine this relation by introducing long chain of inequalities and obtain the trees with the second maximum and the second minimum Harary index. In [29] Zhou, Cai and Trinajstić presented some lower and upper bounds for the Harary index of connected graphs, triangle-free and quadrangle-free graphs and gave the Nordhaus-Gaddum-type inequalities. In [1] the authors obtained some lower and upper bounds for the Harary index of graphs in terms of the diameter and the number of connected components. Zhou, Du and Trinajstić [30] discussed the Harary index of landscape graphs, which have found applications in ecology [?]. Feng and Ilić in [7] establish sharp upper bounds for the Zagreb indices, sharp upper bound for the Harary index and sharp lower bound for the hyper-Wiener index of graphs with a given matching number.

In this paper, we analyze relations between the extremal trees with maximum and minimum Harary and Wiener index. We investigate the Harary index of n-vertex trees with given number of pendent vertices and determine the extremal trees with maximal $H(G)$. Furthermore, we derive the partial ordering of starlike trees based on the majorization inequalities of the pendent path lengths. We characterize the extremal trees with maximal Harary index in terms of the number of vertices of degree two, the matching number, independence number, radius and diameter. Finally, we characterize the extremal trees with minimal Harary index with respect to the maximum vertex degree. All these results are compared with those of the ordinary Wiener index. We conclude the paper by posing a conjecture regarding to the extremal tree with the maximum Harary index among n-vertex trees with fixed maximum degree.

2   Preliminaries

For any two vertices u and v in G, the distance between u and v, denoted by $d_G(u, v)$, is the number of edges in a shortest path joining u and v. The eccentricity $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex. The vertices of minimum eccentricity form the center. A tree has exactly one or two adjacent center vertices; in this latter case one speaks of a bicenter. The diameter $d(G)$ of a graph G is the maximum eccentricity over all vertices in a graph, while the radius $r(G)$ is the minimum eccentricity over all $v \in V(G)$. For a vertex u in G, the degree of u is denoted by $deg(u)$.

Two distinct edges in a graph G are *independent* if they are not incident with a common vertex in G. A set of pairwise independent edges in G is called a *matching* in G, while a matching of maximum cardinality is a *maximum matching* in G. The *matching number* $\beta(G)$ of G is the cardinality of a maximum matching of G. It is well known that $\beta(G) \leq \frac{n}{2}$, with equality

if and only if G has a perfect matching. The *independence number* of G, denoted by $\alpha(G)$, is the size of a maximum independent set of G.

Let P_n and S_n denote the path and the star on n vertices. A *starlike tree* is a tree with exactly one vertex of degree at least 3. We denote by $S(n_1, n_2, \ldots, n_k)$ the starlike tree of order n having a branching vertex v and

$$S(n_1, n_2, \ldots, n_k) - v = P_{n_1} \cup P_{n_2} \cup \ldots \cup P_{n_k},$$

where $n_1 \geq n_2 \geq \ldots \geq n_k \geq 1$. Clearly, the numbers $n_1, n_2, \ldots, n_k$ determine the starlike tree up to isomorphism and $n = n_1 + n_2 + \ldots + n_k + 1$. The starlike tree $BS_{n,k} \cong S(n_1, n_2, \ldots, n_k)$ is *balanced* if all paths have almost equal lengths, i.e., $|n_i - n_j| \leq 1$ for every $1 \leq i < j \leq k$.

Denote by $\Delta(T)$ the maximum vertex degree of a tree T. The path P_n is the unique tree with $\Delta = 2$; while the star S_n is the unique tree with $\Delta = n - 1$. Therefore, we can assume that $3 \leq \Delta \leq n - 2$. The broom $B_{n,\Delta}$ is a tree consisting of a star $S_{\Delta+1}$ and a path of length $n - \Delta - 1$ attached to an arbitrary pendent vertex of the star.

If $\frac{n-1}{2} < m \leq n-1$, then $A_{n,m}$ is the tree obtained from S_{m+1} by adding a pendent edge to each of $n - m - 1$ of the the pendent vertices of S_{m+1}. We call $A_{n,m}$ a *spur* (see Fig. 1). Clearly, $A_{n,m}$ has n vertices and m pendent vertices; the matching number and the independence number of $A_{n,m}$ are $n - m$ and m, respectively. Note that if $m > \frac{n-1}{2}$, then $A_{n,m} \cong BS_{n,m}$.
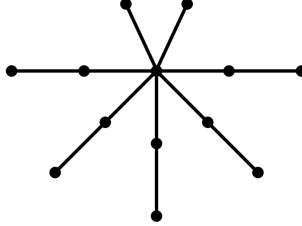

Figure 1:   *The spur* $A_{13,7}$.

Next, we give some lemmas which are very useful in the following.

Definition 2.1 *Let v be a vertex of a tree T and $deg(v) = m + 1$. Suppose that $P_1, P_2, \ldots, P_m$ are pendent paths incident with v, with the starting vertices of paths $v_1, v_2, \ldots, v_m$, respectively and lengths $n_i \geq 1$ ($i = 1, 2, \ldots, m$). Let w be the neighbor of v distinct from v_i. Let $T' = \delta(T, v)$ be a tree obtained from T by removing the edges $vv_1, vv_2, \ldots, vv_{m-1}$ and adding edges $wv_1, wv_2, \ldots, wv_{m-1}$. We say that T' is a δ-transform of T.*

This transformation preserves the number of pendent vertices in a tree T.

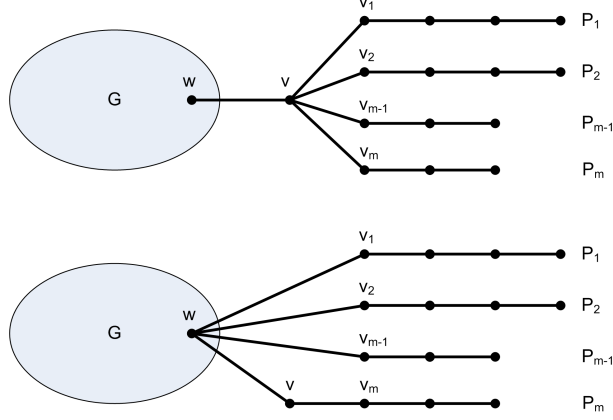Figure 2: δ-transformation on vertex v.

Lemma 2.2 *Let T be a tree rooted at the center vertex u with at least two vertices of degree 3. Let $v \in \{z| \ deg(z) \geq 3, z \neq u\}$ be a vertex with the largest distance $d(u,v)$ from the center vertex. Then for the δ-transformation tree $T' = \delta(T, v)$, it holds*

$$H(T') > H(T).$$

Proof. We follow the symbols in Definition 2.1. Let G be the component of $T - wv$ containing the vertex w (as shown in Fig. 3). Let $R = \{P_1, P_2, \ldots, P_{m-1}\}$. After δ-transformation, the distances between vertices from G and R decreased by 1, while the distances between vertices from R and $Q = P_m \cup \{v\}$ increased by 1. By direct calculation, we have

$$H(T') - H(T) = \sum_{x \in G, y \in R} \frac{1}{d(x,y) - 1} - \frac{1}{d(x,y)} + \sum_{x \in Q, y \in R} \frac{1}{d(x,y) + 1} - \frac{1}{d(x,y)}.$$

According to the assumption, there is an induced path $P = w w_1 w_2 \ldots w_k$ in G, with length at least $\max\{n_1, n_2, \ldots, n_m\}$. For each path P_i, $1 \leq i \leq m - 1$, it follows

$$
\begin{aligned}
D_i \ &= \ \sum_{x \in G, y \in P_i} \left(\frac{1}{d(x,y) - 1} - \frac{1}{d(x,y)} \right) + \sum_{x \in Q, y \in P_i} \left(\frac{1}{d(x,y) + 1} - \frac{1}{d(x,y)} \right) \\
&> \ \sum_{x \in P, y \in P_i} \left(\frac{1}{d(x,y) - 1} - \frac{1}{d(x,y)} \right) - \sum_{x \in Q, y \in P_i} \left(\frac{1}{d(x,y)} - \frac{1}{d(x,y) + 1} \right) \\
&\geq \ 0.
\end{aligned}
$$

5

Hence

$$H(T') - H(T) = \sum_{i=1}^{m-1} D_i > 0.$$

Since T contains at least two vertices of degree at least 3, we have strict inequality. Therefore, if we move pendent paths P_i towards the center vertex u of T along the path P, the Harary index increases. ■

Lemma 2.3 *[10] Let G be a connected graph and $v \in V(G)$. Suppose that $P = v_0v_1 \ldots v_k, Q = u_0u_1 \ldots u_m$ are two paths with lengths k and m ($k \geq m \geq 1$), respectively. Let $G_{k,m}$ be the graph obtained from G, P, Q by identifying v with v_0, u with u_0, respectively. Then*

$$H(G_{k,m}) > H(G_{k+1,m-1}).$$

By Lemma 2.2 and Lemma 2.3, we can get the following

Proposition 2.4 *Let G_0 be a connected graph and $u \in V(G_0)$. Assume that G_1 is the graph obtained from G_0 by attaching a tree T ($T \not\cong P_k$ and $T \not\cong S_k$) of order k to u; G_2 is the graph obtained from G_0 by identifying u with an endvertex of a path P_k; G_3 is the graph obtained from G_0 by identifying u with the center of a star S_k. Then*

$$H(G_2) < H(G_1) < H(G_3).$$

Let $x = (x_1, x_2, \ldots, x_n)$ and $y = (y_1, y_2, \ldots, y_n)$ be two integer arrays of length n. We say that x majorizes y and write $x \succ y$ if the elements of these arrays satisfy following conditions:

(i) $x_1 \geqslant x_2 \geqslant \ldots \geqslant x_n$ and $y_1 \geqslant y_2 \geqslant \ldots \geqslant y_n$,

(ii) $x_1 + x_2 + \ldots + x_k \geqslant y_1 + y_2 + \ldots + y_k$, for every $1 \leqslant k < n$,

(iii) $x_1 + x_2 + \ldots + x_n = y_1 + y_2 + \ldots + y_n$.

Theorem 2.5 *Let $p = (p_1, p_2, \ldots, p_k)$ and $q = (q_1, q_1, \ldots, q_k)$ be two arrays of length $k \geqslant 2$, such that $p \prec q$ and $n = p_1 + p_2 + \ldots + p_k = q_1 + q_2 + \ldots q_k$. Then*

$$H(S(p_1, p_2, \ldots, p_k)) \geq H(S(q_1, q_2, \ldots, q_k)). \tag{1}$$

Proof. We will proceed by induction on the size of the array k. For $k = 2$, we can directly apply transformation from Lemma 2.3 on tree $S(q_1, q_2)$ several times, in order to get $S(p_1, p_2)$. Assume that the inequality (1) holds for all lengths less than or equal to k. If there exist an index $1 \leqslant m < k$ such that $p_1 + p_2 + \ldots + p_m = q_1 + q_2 + \ldots + q_m$, we can apply the induction

6

hypothesis on two parts $S(q_1, q_2, \ldots, q_m) \cup S(q_{m+1}, q_{m+2}, \ldots, q_k)$ and get $S(p_1, p_2, \ldots, p_m) \cup S(p_{m+1}, p_{m+2}, \ldots, p_k)$.

Otherwise, we have strict inequalities $p_1 + p_2 + \ldots + p_m < q_1 + q_2 + \ldots + q_m$ for all indices $1 \leqslant m < k$. We can transform tree $S(q_1, q_2, \ldots, q_k)$ into

$$S(q_1, q_2, \ldots, q_{s-1}, q_s - 1, q_{s+1}, \ldots, q_{r-1}, q_r + 1, q_{r+1}, \ldots, q_k),$$

where s is the largest index such that $q_1 = q_2 = \ldots = q_s$ and r is the smallest index such that $q_r = q_{r+1} = \ldots = q_k$. The condition $p \prec q$ is preserved, and we can continue until the array q transforms into p, while at every step we increase the Harary index. ∎

Corollary 2.6 *Let $T = S(n_1, n_2, \ldots, n_k)$ be a starlike tree with n vertices and k pendent paths. Then*

$$H(B_{n,k}) \leq H(T) \leq H(BS_{n,k}).$$

The left equality holds if and only if $T \cong B_{n,k}$ and the right equality holds if and only if $T \cong BS_{n,k}$.

3 Main results

3.1 Trees with given number of pendent vertices

Let $\mathcal{T}_{n,k}$ $(2 \leq k \leq n-1)$ be the set of trees on n vertices with k pendent vertices. If $k = 2$, then the tree is just the path P_n. If $k = n-1$, then the tree is just the star S_n. Therefore, we can assume that $3 \leq k \leq n-2$ in the sequel. It was proved in [13] that among n-vertex trees with given number k of pendent vertices or given number q of vertices of degree two, $BS_{n,k}$ and $BS_{n,n-q-q}$ have minimal Wiener index.

Theorem 3.1 *Of all the trees on n vertices with k $(3 \leq k \leq n-2)$ pendent vertices, $BS_{n,k}$ is the unique tree having maximal Harary index.*

Proof. Suppose $T \in \mathcal{T}_{n,k}$ has the maximal Harary index, rooted at the center vertex. Let $S_T = \{v \in V(T) : deg(v) \geq 3\}$.

If $|S_T| = 1$, then by Corollary 2.6, it follows that $BS(n, k)$ is the unique tree that maximizes Harary index. If $|S_T| \geq 2$, then there must exist at least two vertices of degree at least 3 and there are only pendent paths attached below them. We can consider T as the rooted tree at the center vertex, and choose the vertex v of degree at least 3 that is furthest from the center vertex. After applying δ-transformation, we increase $H(G)$ while keeping the number of pendent vertices fixed – which is contradiction. ∎

Theorem 3.2 *Among trees with fixed number q $(0 \le q \le n-1)$ of vertices of degree two, $T_{n,n-1-q}$ is the unique tree having maximal Harary index.*

Proof. The proof is similar to that of Theorem 3.1.

Consider δ-transformed tree $T' = \delta(T, v)$. The vertex v has degree greater than two, while the vertex w has degree greater than or equal to two. Among vertices on the pendent paths $P_1, P_2, \ldots, P_m$, there are

$$S = (n_1 - 1) + (n_2 - 1) + \ldots + (n_m - 1) = \sum_{i=1}^{m} n_i - m$$

vertices of degree two.

If w has degree two in T, then after δ-transformation, v will have degree two, and the number of vertices of degree two in T' remains the same as in T. Otherwise, assume that $deg(w) > 2$. We can apply one transformation from Lemma 2.3, and get new tree T'' with $m+1$ pendent paths attached at vertex w with lengths $n_1, n_2, \ldots, n_m, 1$. This way we increased Harary index, while the number of vertices with degree two in trees T and T'' are the same.

By repetitive application of these transformations, we prove that the starlike tree has maximal value of Harary index among trees with q vertices of degree two. The number of pendent paths is exactly $k = \sum_{i=1}^{m} n_i - q = n - 1 - q$, and by Corollary 2.6 it follows that balanced starlike tree $BS(n, n-1-q)$ is the unique tree that maximizes Harary index. ∎

By Lemma 2.3, we have the following chain of inequalities

$$H(P_n) = H(BS_{n,2}) < H(BS_{n,3}) < \ldots < H(BS_{n,n-1}) = H(S_n). \qquad (2)$$

Notice that Lemma 2.2 from [1], $H(P_n) \le \frac{(n+2)(n-1)}{4} = H(S_n)$ follows directly from these inequalities.

3.2 Trees with given matching or independence number

Du and Zhou in [6] proved that among n-vertex trees with given matching number m, the spur $A_{n,m}$ minimizes the Wiener index.

Lemma 3.3 *For arbitrary $\frac{n-1}{2} \le m \le n-1$, there holds*

$$H(A_{n,m}) = \frac{1}{24} \left(3n^2 + 2mn + m^2 - 9m + 19n - 22 \right).$$

Proof. There are four types of vertices in the tree $A_{n,m}$. Denote with $D'(v)$ the sum of all reverse distances from v to all other vertices.

- For the center vertex, $D'(v) = \frac{m}{1} + \frac{n-m-1}{2}$;

- For each pendant vertex attached to the center vertex, $D'(v) = \frac{1}{1} + \frac{m-1}{2} + \frac{n-m-1}{3}$;

- For each vertex of degree 2, different from the center vertex, $D'(v) = \frac{2}{1} + \frac{m-1}{2} + \frac{n-m-2}{3}$;

- For each pendant vertex not attached to the center vertex, $D'(v) = \frac{1}{1} + \frac{1}{2} + \frac{m-1}{3} + \frac{n-m-2}{4}$.

After summing above contributions to the Harary index, we get

$$
\begin{aligned}
H(A_{n,m}) &= 1 \cdot \frac{n+m-1}{2} + (2m-n+1) \cdot \frac{2n+m+1}{6} \\
&\quad + (n-m-1) \cdot \frac{2n+m+5}{6} + (n-m-1) \cdot \frac{3n+m+8}{12} \\
&= \frac{1}{24} \left(3n^2 + m^2 - 22 - 9m + 19n + 2mn \right).
\end{aligned}
$$

This proves the results. ∎

Theorem 3.4 *Let T be a tree on n vertices with matching number β. Then*

$$
H(T) \leq \frac{1}{24} \left(6n^2 - 4\beta n + \beta^2 + 9\beta + 10n - 22 \right),
$$

with equality holding if and only if $T \cong A_{n,n-\beta}$.

Proof. Suppose that T has k pendent vertices, then

$$
k \leq \beta + n - 2\beta = n - \beta,
$$

and by Theorem 3.1, we have $H(T) \leq H(BS_{n,k})$. Using equation (2), it follows $H(BS_{n,k}) \leq H(BS_{n,n-\beta}) = H(A_{n,n-\beta})$ since $n - \beta \geq \frac{n}{2}$. Finally, $H(T) \leq H(A_{n,n-\beta})$, with equality holding if and only if $T \cong A_{n,n-\beta}$. By Lemma 3.3, we obtain the explicit relation for $H(A_{n,n-\beta})$. ∎

By Theorem 3.4, we have the following corollary.

Corollary 3.5 *Let T be a tree of order n with perfect matching. Then*

$$
H(T) \leq \frac{1}{4}(17n^2 + 58n - 88),
$$

with equality holding if and only if $T \cong A_{n,\frac{n}{2}}$.

Theorem 3.6 *Let T be a tree on n vertices with independence number α. Then*

$$H(T) \le \frac{1}{24} \left(3n^2 + 2\alpha n + \alpha^2 - 9\alpha + 19n - 22\right),$$

with equality holding if and only if $T \cong A_{n,\alpha}$.

Proof. Since all pendent vertices form an independent set, it follows $k \le \alpha$. Every tree is bipartite graph, and we get $\alpha \ge \lceil \frac{n}{2} \rceil$. By Theorem 3.1, we have $H(T) \le H(BS_{n,k})$ and $H(BS_{n,k}) \le H(BS_{n,\alpha}) = H(A_{n,\alpha})$. Therefore, $H(T) \le H(A_{n,\alpha})$, with equality holding if and only if $T \cong A_{n,\alpha}$. $\blacksquare$

3.3   Trees with given diameter or radius

Let $C_{n,d}(p_1, p_2, \ldots, p_{d-1})$ be a caterpillar on n vertices obtained from a path $P_{d+1} = v_0 v_1 \ldots v_{d-1} v_d$ by attaching $p_i \ge 0$ pendant vertices to v_i, $1 \le i \le d-1$, where $n = d + 1 + \sum_{i=1}^{d-1} p_i$. Denote

$$C_{n,d,i} = C_{n,d}(\underbrace{0, \ldots, 0}_{i-1}, n - d - 1, 0 \ldots, 0).$$

Obviously, $C_{n,d,i} = C_{n,d,n-i}$. In [14] and [19] it is shown that caterpillar $C_{n,d,\lfloor d/2 \rfloor}$ has maximal Wiener index among trees with fixed diameter d.

Theorem 3.7 *Among trees on n vertices and diameter d, $C_{n,d,\lfloor d/2 \rfloor}$ is the unique tree having maximal Harary index.*

Proof. Let T be n-vertex tree with diameter d having maximal Harary index. Let $P_{d+1} = v_0 v_1 \ldots v_d$ be a path of length d. By Proposition 2.4, all trees attached to the path P_{d+1} must be stars, which implies that $T \cong C_{n,d}(p_1, p_2, \ldots, p_{d-1})$. Applying Lemma 2.2 at those vertices of degree at least 3 in $C_{n,d}(p_1, p_2, \ldots, p_{d-1})$, we get that $T \cong C_{n,d,i}$ for some $1 \le i \le d-1$. By Lemma 2.3 we get that the maximal Harary index is achieved uniquely for $i = \lfloor \frac{n}{2} \rfloor$. This completes the proof. $\blacksquare$

For a tree T with radius $r(T)$, it holds $2r(T) = d(T)$ or $2r(T) - 1 = d(T)$. Using transformation from Lemma 2.3 applied to a center vertex, it follows that $H(C_{n,2r,\lfloor d/2 \rfloor}) < H(C_{n,2r-1,\lfloor d/2 \rfloor})$.

Corollary 3.8 *Let T be a tree on n vertices with radius $r \ge 2$. Then*

$$H(T) \le H(C_{n,2r-1,\lfloor d/2 \rfloor}),$$

with equality if and only if $T \cong C_{n,2r-1,\lfloor d/2 \rfloor}$.

If $d > 2$, we can apply the transformation from Lemma 2.3 at the center vertex in $C_{n,d,\lfloor d/2 \rfloor}$ to obtain $C_{n,d-1,\lfloor (d-1)/2 \rfloor}$. Thus,

$$H(P_n) = H(C_{n,n-1,\lfloor (n-1)/2 \rfloor}) < \ldots < H(C_{n,3,1}) < H(C_{n,2,1}) = H(S_n).$$

Also, it follows that $H(C_{n,3,1})$ has the second maximum Harary index among trees on n vertices.

3.4 Trees with given maximum vertex degree

Chemical trees (trees with maximum vertex degree at most four) provide the graph representations of alkanes [11]. It is therefore a natural problem to study trees with bounded maximum degree. It was proven in [5] that among n-vertex trees with the maximum degree Δ, the broom $B_{n,\Delta}$ has maximal Wiener index.

Lemma 3.9 *For arbitrary* $2 \leq \Delta \leq n - 1$, *there holds*

$$H(B_{n,\Delta}) = n \cdot H_{n-\Delta} - n + \Delta + \frac{(\Delta - 1)(\Delta - 2)}{4} + \frac{\Delta - 1}{n - \Delta + 1},$$

where $H_k = 1 + \frac{1}{2} + \ldots + \frac{1}{k}$ *be the k-th harmonic number.*

Proof. The Harary index of $B_{n,\Delta}$ can be calculated as the sum of Harary index of $P_{n-\Delta+1}$, the sum of reverse distances between $\Delta - 1$ pendent vertices and vertices from a long path, and the sum of reverse distance between pendent vertices.

$$
\begin{aligned}
H(B_{n,\Delta}) &= H(P_{n-\Delta+1}) + \frac{\binom{\Delta-1}{2}}{2} + (\Delta - 1)H_{n-\Delta+1} \\
&= n \cdot H_{n-\Delta} - n + \Delta + \frac{(\Delta - 1)(\Delta - 2)}{4} + \frac{\Delta - 1}{n - \Delta + 1}.
\end{aligned}
$$

∎

Theorem 3.10 *Let T be a tree on n vertices with the maximum degree Δ. Then $H(T) \leq H(B_{n,\Delta})$. The equality holds if and only if $T \cong B_{n,\Delta}$.*

Proof. Fix a vertex v of degree Δ as a root and let $T_1, T_2, \ldots, T_\Delta$ be the trees attached at v. By Proposition 2.4, all subtrees attached to u_i are paths for $1 \leq i \leq \Delta$, the Harary index increases. This implies the result.
∎

If $\Delta > 2$, we can apply the transformation from Lemma 2.3 at the vertex of degree Δ in $B_{n,\Delta}$ and obtain $B_{n,\Delta-1}$. Thus,

$$H(S_n) = H(B_{n,n-1}) > H(B_{n,n-2}) > \ldots > H(B_{n,3}) > H(B_{n,2}) = H(P_n).$$

Also, it follows that $B_{n,3}$ has the second minimum Harary index among trees on n vertices.

4 Concluding remarks

In this paper, we presented the partial ordering of starlike trees based on the Harary index and we derived the trees with the second maximal and the second minimal Harary index. We characterized the extremal trees with maximal Harary index and fixed number of pendent vertices, the number of vertices of degree two, matching number, independence number, radius and diameter. In addition, we characterized the extremal trees with minimal Harary index and given maximum degree. We concluded that in the all presented classes, the trees with maximum values of Harary index are exactly those trees with the minimal Wiener index $W(G)$, and vice versa.

The complete Δ-ary tree is defined as follows. Start with the root having Δ children. Every vertex different from the root, which is not in one of the last two levels, has exactly $\Delta - 1$ children. In the last level, while not all nodes have to exist, the nodes that do exist fill the level consecutively. Thus, at most one vertex on the level second to last has its degree different from Δ and 1.

In [12] the authors proposed these trees to be called *Volkmann trees*, as they represent alkanes with minimal Wiener index [8]. The computer search among trees with up to 24 vertices reveals that the complete Δ-ary trees attain the maximum values of $H(G)$ among the trees with the maximum vertex degree Δ.

Conjecture 4.1 *For any $k \geqslant 2$, the complete Δ-ary tree has maximum value of $H(G)$ among trees on n vertices with maximum degree Δ.*

It would be interesting for further research to consider the extremal unicyclic and bicyclic graphs with respect to Harary index, and compare the results with those for the Wiener index.

References

[1] K. C. Das, B. Zhou, N. Trinajstić, *J. Math. Chem.* 2010, 46, 1377.

[2] J. Devillers, A.T. Balaban (eds), *Topological indices and related descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, 1999.

[3] M. V. Diudea, *J. Chem. Inf. Comput. Sci.* 1997, 37, 292.

[4] M. V. Diudea, T. Ivanciuc, S. Nikolić, N. Trinajstić, *MATCH Commun. Math. Comput. Chem.* 1997, 35, 41.

[5] A. Dobrynin, R. Entringer, I. Gutman, *Acta Appl. Math.* 2001, 66, 211.

[6] Z. Du, B. Zhou, *MATCH Commun. Math. Comput. Chem.* 2010, 63, 101.

[7] L. Feng, A. Ilić, Zagreb, *Appl. Math. Lett.* 2010, 23, 943.

[8] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Székely, L. Volkmann, *Discrete Appl. Math.* 2002, 122, 127.

[9] X. Guo, D. J. Klein, W. Yan, Y. N. Yeh, *Int. J. Quantum. Chem.* 2006, 106, 1756.

[10] I. Gutman, *Indian J. Chem.* 1997, 36A, 128.

[11] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[12] I. Gutman, B. Furtula, V. Marković, B. Glišić, *Z. Naturforsch.* 2007, 62A, 495.

[13] A. Ilić, M. Ilić, *Linear Algebra Appl.* 2009, 431, 2195.

[14] A. Ilić, A. Ilić, D. Stevanović, *MATCH Commun. Math. Comput. Chem.* 2010, 63, 91.

[15] O. Ivanciuc, T.S. Balaban, A. T. Balaban, *J. Math. Chem.* 1993, 12, 309.

[16] O. Ivanciuc, T. Ivanciuc, A. T. Balaban, *J. Chem. Inf. Comput. Sci.* 1998, 38, 395.

[17] O. Ivanciuc, *J. Chem. Inf. Comput. Sci.* 2000, 40, 1412.

[18] D. Janežić, A. Miličević, S. Nikolić, N. Trinajstić, *Graph Theoretical Matrices in Chemistry, Mathematical Chemistry Monographs No. 3*, University of Kragujevac, Kragujevac, 2007.

[19] H. Liu, X. F. Pan, *MATCH Commun. Math. Comput. Chem.* 2008, 60, 85.

[20] B. Lučić, I. Lukovits, S. Nikolić, N. Trinajstić, *J. Chem. Inf. Comput. Sci.* 2001, 41, 527.

[21] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, *Croat. Chem. Acta* 2002, 75, 847.

[22] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, *J. Math. Chem.* 1993, 12, 235.

[23] R. Todeschini, V. Consonni, *Handbook of molecular descriptors*, Wiley-VCH, Weinheim, 2000, pp. 209–212.

[24] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009, pp. 371–375.

[25] N. Trinajstić, S. Nikolić, S. C. Basak, I. Lukovits, *SAR QSAR Environ. Res.*, 2001, 12, 31.

[26] D. Urban, T. Keitt, *Ecology* 2001, 82, 1205.

[27] B. Zhou, *Int. J. Quantum Chem.* 2006, 107, 875.

[28] B. Zhou, N. Trinajstić, *Int. J. Quantum Chem.* 2008, 108, 858.

[29] B. Zhou, X. Cai, N. Trinajstić, *J. Math. Chem.* 2008, 44, 611.

[30] B. Zhou, Z. Du, N. Trinajstić, *Int. J. Chem. Model.* 2008, 1, 35.